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Table S1. Crystal and Refinement Data

crystal system	tetragonal
space group	$P\ \bar{4}n2$ (No. 118)
formula	$C_{13}H_{32}Cl_2CuN_4O_8$
a, Å	9.1203(6)
c, Å	13.0859(9)
V, Å^3	1088.5(1)
ρ_{calcd}, g cm^{-3}	1.547
fw	506.87
Z	2
μ, cm^{-1}	12.94
temp, K	296
λ, Å	0.71073
independent reflcns	3697
obseved reflcns ($F_o > 2\sigma$)	2126
transmission coefficients, $A_{max, min}$	1.104, 1.000
index ranges	$0 \le h \le 10$, $-10 \le k \le 10$, $-15 \le l \le 15$
crystal size	0.30 × 0.30 × 0.20 mm
crystal habit	blue prism
refinement method	full-matrix least-squares
$2\theta_{max}$, deg	50
Data, restraints, parameters	3697, 25, 77
Goodness of fit on F^2	1.072
residual extrema, e Å^{-3}	+0.56, -0.44
$R(F_o)^a$, $wR_2(F_o^2)^b$	0.0632, 0.1735

^{a} $R(F_o) = \sum ||F_o| - |F_c|| \sum |F_o|$, ^{b} $wR_2(F_o^2) = (\sum w(F_o^2 - F_c^2) / \sum wF_o^2)^{1/2}$

$w = (\sigma^2(F_o^2) + (0.1331P)^2 + 0.04P)^{-1}$, where $P = \frac{1}{3} \max(F_o^2,0) + \frac{2}{3}F_c^2$.

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($A^2 \times 10^3$) for $[CuL^1(OClO_3)_2]$. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Cu	5000	0	2500	76(1)
N(1)	6180(17)	1351(16)	1556(7)	101(4)
N(2)	5800(14)	867(17)	3904(6)	107(3)
C(1)	7848(33)	847(41)	1480(30)	200(12)
C(2)	7354(13)	474(15)	4100(9)	87(3)
C(3)	5000	0	294(9)	157(3)
C(4)	4921(20)	1632(19)	630(14)	134(5)
C(5)	6430(24)	2884(23)	1816(16)	144(6)
C(6)	6970(27)	2570(30)	2979(15)	108(8)
C(7)	6029(36)	2430(39)	4034(26)	217(17)
Cl	1889(2)	3111(2)	2500	148(1)
O(1)	3013(5)	1987(5)	2500	158(2)
O(2)	584(18)	2564(21)	1957(15)	199(7)
O(3)	2486(13)	4198(13)	1675(9)	130(3)
O(4)	1754(17)	3743(16)	3299(10)	186(6)

Table S3. Bond lengths [Å] and angles [deg] for $[CuL^1(OClO_3)_2]$.

Cu-N(1)	2.050(7)
Cu-N(2)	2.129(8)
Cu-O(1)	2.562(7)
N(1)-C(5)	1.46(3)
N(1)-C(1)	1.59(4)
N(1)-C(4)	1.69(2)
N(2)-C(7)	1.45(4)
N(2)-C(2)	1.48(2)
N(2)-C(3)#1	1.504(13)
C(3)-C(4)	1.55(2)
C(5)-C(6)	1.62(2)
C(6)-C(7)	1.63(2)
Cl-O(1)	1.450(7)
Cl-O(2)	1.47(2)
Cl-O(3)	1.564(11)
Cl-O(4)	1.201(14)

N(1)-Cu-N(1)#2	173.8(11)
N(1)-Cu-N(2)#2	83.2(5)
N(1)-Cu-N(2)	96.7(5)

N(2)#2-Cu-N(2)	177.7(9)
N(1)-Cu-O(1)	86.9(5)
N(2)-Cu-O(1)	88.8(5)
C(5)-N(1)-C(1)	98(2)
C(5)-N(1)-C(4)	97.4(14)
C(1)-N(1)-C(4)	130(2)
C(5)-N(1)-Cu	121.2(11)
C(1)-N(1)-Cu	112(2)
C(4)-N(1)-Cu	99.6(8)
C(7)-N(2)-C(2)	95(2)
C(7)-N(2)-C(3)#1	120(2)
C(2)-N(2)-C(3)#1	102.4(12)
C(7)-N(2)-Cu	121(2)
C(2)-N(2)-Cu	112.7(8)
C(3)#1-N(2)-Cu	103.9(6)
N(2)#2-C(3)-C(4)	104.0(11)
C(3)-C(4)-N(1)	91.5(10)
N(1)-C(5)-C(6)	96(2)
C(5)-C(6)-C(7)	130(2)
N(2)-C(7)-C(6)	93(2)
O(4)-Cl-O(1)	114.3(6)
O(4)-Cl-O(2)	120.0(9)

O(1)-Cl-O(2)	109.4(7)
O(4)-Cl-O(3)	109.4(9)
O(1)-Cl-O(3)	101.7(4)
O(2)-Cl-O(3)	99.4(7)

Symmetry transformations used to generate equivalent atoms:

#1 y+1/2,x-1/2,-z+1/2 #2 -y+1/2,-x+1/2,-z+1/2

Table S4. Anisotropic displacement parameters ($Å^2 \times 10^3$) for $[CuL^1(OClO_3)_2]$.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [h^2 a^{*2} U11 + ... + 2 h k a^* b^* U12]$

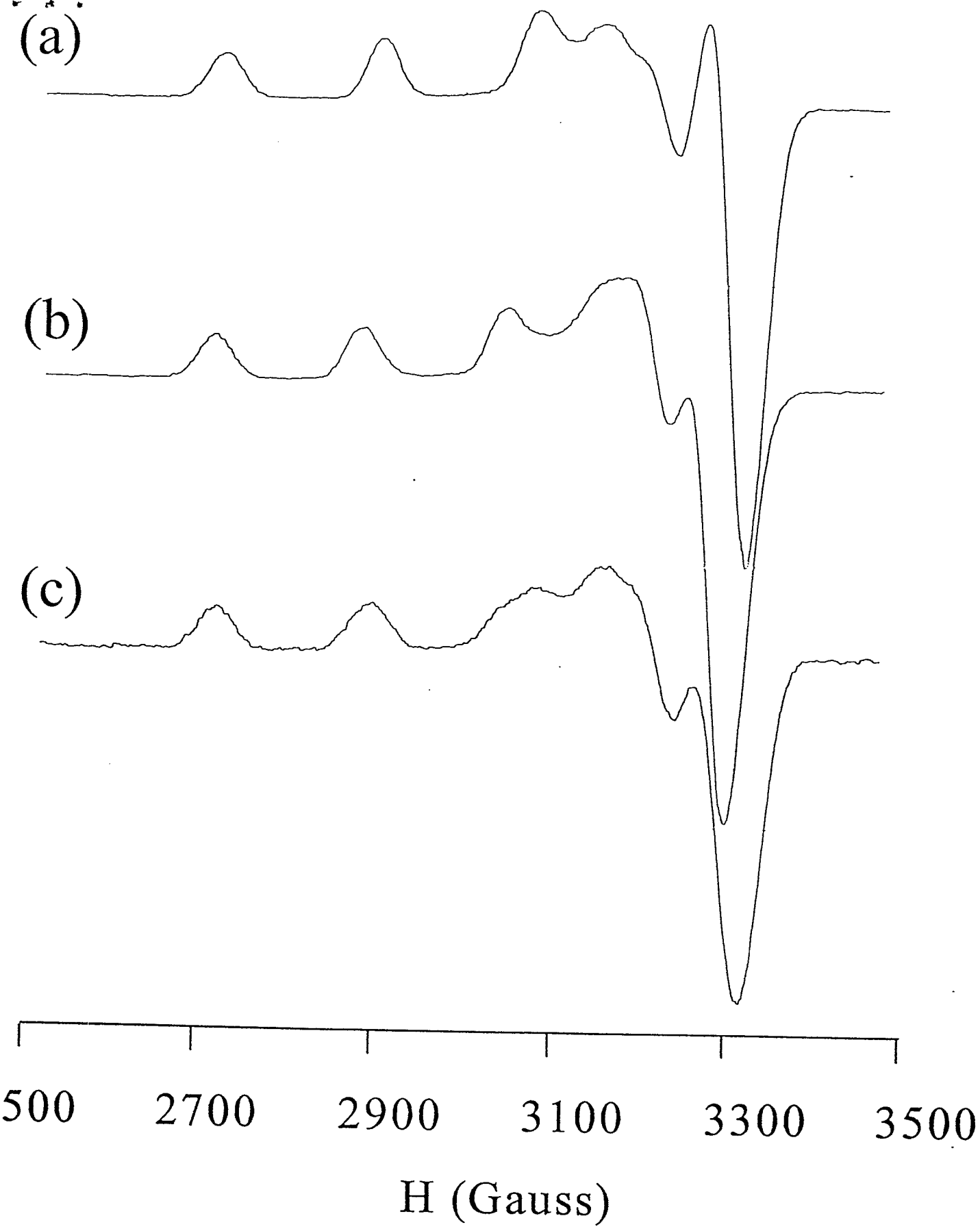
	U11	U22	U33	U23	U13	U12
Cu	91(1)	91(1)	46(1)	0	0	-12(1)
N(1)	142(13)	72(7)	90(5)	-15(7)	24(8)	-30(5)
N(2)	75(9)	164(14)	81(5)	-34(7)	28(7)	-15(6)
C(2)	94(7)	95(7)	72(6)	-4(5)	-45(5)	-18(6)
C(6)	94(14)	121(17)	108(13)	-12(10)	9(10)	31(15)
Cl	165(1)	165(1)	114(1)	-16(3)	-16(3)	53(2)

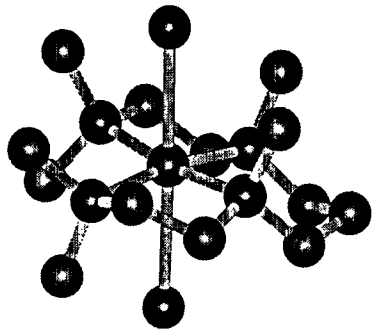
Table S5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for $[CuL^1(OClO_3)_2]$.

	x	y	z	U(eq)
H(1A)	7934(33)	-159(41)	1272(30)	260
H(1B)	8290(33)	971(41)	2140(30)	260
H(1C)	8338(33)	1463(41)	992(30)	260
H(2A)	7437(13)	-570(15)	4025(9)	113
H(2B)	7626(13)	748(15)	4783(9)	113
H(2C)	7994(13)	949(15)	3621(9)	113
H(3A)	4229	-651	527(9)	204
H(3B)	5475	-269	-343(9)	204
H(4A)	3957(20)	1933(19)	863(14)	175
H(4B)	5268(20)	2280(19)	95(14)	175
H(5A)	5557(24)	3492(23)	1820(16)	187
H(5B)	7214(24)	3355(23)	1438(16)	187
H(6A)	7761(27)	3213(30)	3189(15)	140
H(6B)	7401(27)	1607(30)	2886(15)	140
H(7A)	6453(36)	2774(39)	4670(26)	282
H(7B)	5066(36)	2853(39)	3923(26)	282

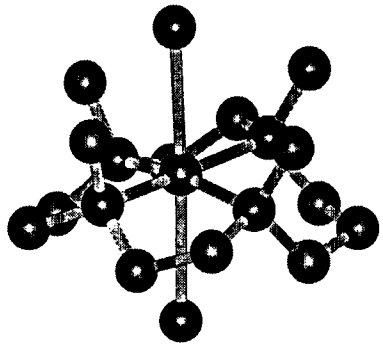
Figure S1. X-Band (9.278 GHz) EPR spectra of (a) $[CuL^4](ClO_4)_2$, (b) $[CuL^1](ClO_4)_2$ and (c) the co-crystallized mixture of $[CuL^4](ClO_4)_2$ and $[CuL^1](ClO_4)_2$ (H_2O:DMF 2:1, 77 K).

Figure S2. Molecular mechanics predicted geometries and strain energies of the three non-degenerate conformations of $[CuL^1(OH_2)_2]^{2+}$ (a) $\delta\lambda$, (b) $\lambda\delta$ and (c) $\delta\delta$ (H-atoms omitted).

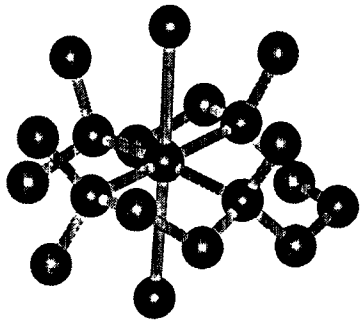

(a)
(b)
(c)
500
2700
2900
3100
3300
3500
H (Gauss)



(a) 74.99 kJ mol^{-1}



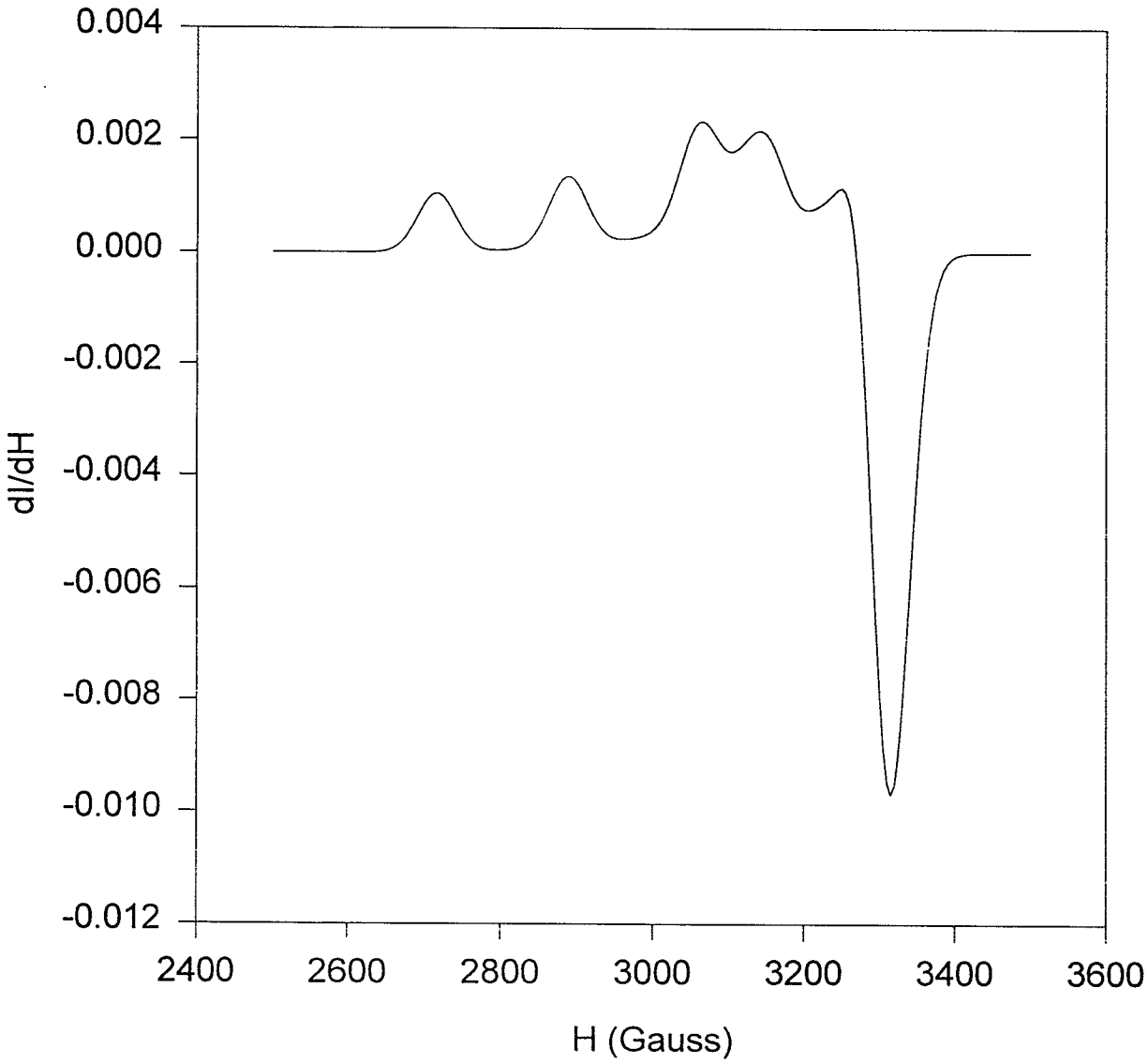
(b) 92.69 kJ mol^{-1}



(c) 77.99 kJ mol^{-1}

[CuL^1]$^{2+}$ - simulated EPR spectrum

$g_{||}$ 2.228 $A_{||}$ 172 G $g_{\perp}$ 2.054 $A_{\perp}$ 30 G



$[CuL^4]^{2+}$ - simulated EPR spectrum

$g_{||}$ 2.205 $A_{||}$184 G $g_{\perp}$ 2.045 $A_{\perp}$ 30 G